数学与系统科学研究院

计算数学所学术报告

报告人：**Dr Christian Mendl**

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报告题目：

Numerical methods for a Kohn-Sham density functional model based on optimal transport

邀请人：　　周爱辉 研究员

报告时间：**2014** 年 **10** 月 **30** 日（周四）

上午 **10:00-11:00**

报告地点：　　数学院南楼六层 **602** 会议室

Abstract:

The talk is concerned with numerical discretizations to solve density functional models in the "strictly correlated electrons" (SCE) framework. In the SCE framework, the exchange-correlation functional encodes the effects of the strong correlation regime by minimizing the pairwise Coulomb repulsion, resulting in an optimal transport problem. We construct an efficient numerical discretization for this type of problem for N = 2 electrons and apply it to the H2 molecule in its dissociating limit.

欢迎大家参加！